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Chapter 1

Introduction

1.1 Differential Equations

Differential equations are important mathematical tools central to the investigations carried out in many branches of science and technology. Mathematical modeling of diverse physical phenomena often consists of systems of differential equations. Differential equations are broadly divided into (a) ordinary differential equations or ODEs and (b) partial differential equations or PDEs.

Definition 1.1.1. *An **ordinary differential equation** is an equation in an unknown function $y = y(x)$ of a real variable x, its derivatives $D^n y$ with respect to x, and some arbitrary functions $f_m = f_m(x)$ of x, for $n, m \in \mathbb{N}$. The unknown function y is the **dependent variable** whereas the real variable x is the **independent variable** of the equation. The **order** of the differential equation is the highest value of $n \in \mathbb{N}$ in $D^n y$.*

Partial differential equations involve an unknown function $y = y(x_1, ..., x_n)$ of an independent variable $x = (x_1, ..., x_n)$. The theory of ordinary differential equations is a special case of the more general theory of partial differential equations for $n = 1$. In what follows, we shall be concerned primarily with the former of these two types of differential equations. However, functions of more than one real variable do appear quite frequently.

1.1.1 Initial-Value Problems

Ordinary differential equations encountered in physical problems are often accompanied by initial conditions, thus constituting initial-value problems or IVPs. These conditions define the state of the dynamic system at time $x = x_0$. An initial-value problem is generically written as

$$Dy(x) = f(x, y(x)), \;\; y(x_0) = y_0. \tag{1.1.1.1}$$

Here $f(x, y(x))$ is a definite function which depends upon x and $y = (y_1, ..., y_n)$.

A function $y_* = (y_{*1}, ..., y_{*n})$ is a **solution** of (1.1.1.1) if it satisfies the differential equation identically for all $x \in Dom(y_*)$, and the initial condition $y(x_0) = y_0$. The **dimension n of the solution space** for an initial-value problem is defined as the **dimension of the problem**.

We often consider **autonomous IVPs** for which x equals to y_i for some $1 \leq i \leq n$ of the solution $y = (y_1, ..., y_n)$. The resulting differential equation has $f = f(x; y) = f(y_i; y) = f(y_1, ..., y_n) = f(y)$ as function of y only. An autonomous initial-value problem is typically written as

$$Dy = f(y), \;\; y(x_0) = y_0 \tag{1.1.1.2}$$

1.2 Numerical Methods for ODEs

Numerical methods are used to find numerical (approximate) solutions of differential equations. These methods use initial conditions as their starting point. An ordinary differential equation with an initial condition is solved using the initial conditions and moving it along the path specified by the differential equation. Good convergence and stability are desirable characteristics for a numerical method.

There are many methods available for the numerical solution of differential equations of various types and orders. We give numerical methods for the integration of ordinary differential equation only. Methods presented here are: a) the one-step methods b) the multi-step methods and c) general linear methods.

1.2.1 One-Step Methods

One-Step methods are a class of classical numerical methods for the solution of ordinary differential equations. One-Step methods calculate the

approximation y_{n+1} to the exact solution y of a differential equation using the previous approximation y_n only, thus requiring single step information at each of the successive iterations. The one-step methods presented here are a)the Euler method and b) the Runge-Kutta methods.

1.2.2 Euler Method

The Euler method is the simplest of the one-step numerical methods for solution of initial value-problem. They use the tangent line approximation to move from one point to the next along the integral curve at each iteration of the approximation process. Let $h = \triangle x$ be the constant step size, and $f(x, y) = Dy$ represent the slope of the integral curve at point (x, y). The general form for the Euler method is given as

$$x_{n+1} = x_n + h, \;\; y_{n+1} = y_n + hf(x_n, y_n).$$

The Euler method uses the initial condition $y(x_0) = y_0$ as its starting value upon the very first iteration to find later approximations $y_i, \;\; i > 1$. The general form for the **implicit Euler method** is given as

$$y_{n+1} = y_n + hf(x_{n+1}, y_{n+1}). \tag{1.2.2.1}$$

The Euler method is accurate only up to first order.

1.2.3 Runge-Kutta Methods

The Runge-Kutta methods are used to achieve higher order accuracy for the numerical solution of ordinary differential equations. The general form of a Runge-Kutta of order s defined by three sets of parameters $a_{ij}, \;\; 1 \leq i, j \leq s$, b_i and $c_i, \;\; i = 1, ..., s$ is

$$Y_i = y_{n-1} + h\sum_{j=1}^{s} a_{ij} f(Y_j), \;\; y_n = y_{n-1} + h\sum_{i=1}^{r} b_i f(Y_i), \tag{1.2.3.1}$$

Here s and r denote the number of stages and the number of input quantities, respectively. y_{n-1} represent the input quantities at the beginning of

step n, whereas y_n are the output quantities. $Y_i, i = 1, ..., s$ are the stages and $A = (a_{ij})$ denotes an $s \times s$ matrix with b_i and $c_i, i = 1, ..., s$ as quadrature weights.

In Runge-Kutta methods, we first evaluate s-stage values $Y_1, Y_2, ..., Y_s$ and then calculate output values by using linear combinations of their derivatives. The Runge-Kutta methods can be represented by Butcher tableau as [1].

$$\begin{array}{c|ccc} c_1 & a_{11} & \dots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \dots & a_{ss} \\ \hline & b_1 & \dots & b_s \end{array}$$

where the nodes of the method are $c_i = \sum_{j=1}^{s} a_{ij}$ at which the stages Y_i are obtained.

Runge-Kutta methods is known as explicit if $A = [a_{ij}]$ is an upper triangular matrix otherwise they are known as implicit. The classical fourth order explicit Runge-Kutta method is represented using Butcher tableau as

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array}$$

1.2.4 Linear Multi-Step Methods

Linear multi-step methods are important numerical methods for the solution of ordinary differential equations. These methods use more than one value from previous time steps while approximating the solution of an initial

value problem. The standard form of a linear $k-$step method is

$$y_n = \sum_{i=1}^{k} \alpha_i y_{n-i} + h \sum_{i=0}^{k} \beta_i f(y_{n-i}). \tag{1.2.4.1}$$

A starting method is required to start the process because this method used more than one values of solution y in the past. Usually, one-step methods are used as the starting method.

Popular families of linear multi-step methods are Adams-Bashforth methods and Adams-Moulton methods. If we take $\alpha_1 = 1$, $\alpha_i = 0, i \neq 1$, and $\beta_0 = 0$ in the general form of linear multi-step methods, we get

$$y_n = y_{n-1} + h[\beta_1 f(y_{n-1}) + \beta_2 f(y_{n-2}) + ... + \beta_k f(y_{n-k})]. \tag{1.2.4.2}$$

This is the explicit linear multi-step method of order k known as Adams-Bashforth method. Similarly, if instead $\beta_0 \neq 0$, we get

$$y_n = y_{n-1} + h[\beta_0 f(y_n) + \beta_1 f(y_{n-1}) + \beta_2 f(y_{n-2}) + ... + \beta_k f(y_{n-k})] \tag{1.2.4.3}$$

which is the implicit linear multi-step method of order $k + 1$ known as Adams-Moulton method.

1.2.5 General Linear Methods

Generalizing the linear multi-step methods further gives us the important class of numerical methods called *general linear methods*. The idea is to import some of the input quantities at the beginning of a step n and then computing the corresponding stage derivatives $F(y_i)$ and stage values Y_i. Each stage value is a linear combination of y_{n-1} and $F(Y_i)$. The input values are obtained by using the starting method at the initial step $n = 1$.

Suppose that r input quantities are passed on from one step to the next. At the start of step n, these will be denoted by ${y_1}^{[n-1]}, ..., {y_r}^{[n-1]}$,. The

corresponding quantities available for use in the subsequent step will be ${y_1}^{[n]}, ..., {y_r}^{[n]}$. During the computation of the step, we take

$$\begin{aligned} y^{[n-1]} &= \begin{pmatrix} {y_1}^{[n-1]} \\ \vdots \\ {y_r}^{[n-1]} \end{pmatrix}, \quad y^{[n]} = \begin{pmatrix} {y_1}^{[n]} \\ \vdots \\ {y_r}^{[n]} \end{pmatrix}, \\ Y &= \begin{pmatrix} Y_1 \\ \vdots \\ Y_s \end{pmatrix}, \qquad F = \begin{pmatrix} F_1 \\ \vdots \\ F_s \end{pmatrix}. \end{aligned} \tag{1.2.5.1}$$

The general form for a general linear method of order k is given in [7] as,

$$Y_i^{[n]} = \sum_{j=1}^{s} hAf(Y_j^{[n]}) + \sum_{j=1}^{r} Uy_j^{[n-1]}, \;\; i = 1, ..., s \tag{1.2.5.2}$$

$$y_i^{[n]} = \sum_{j=1}^{s} hBf(Y_j^{[n]}) + \sum_{j=1}^{r} Vy_j^{[n-1]}, \;\; i = 1, ..., r. \tag{1.2.5.3}$$

Here s and r denote the number of stage values and the number of input quantities, respectively. $Y_i^{[n]} \approx y(t_n + c_i h), \;\; i = 1, ..., s$ is the stage value calculated at step n, and $F_i = f(Y_i^{[n]}) \;\; i = 1, ..., s$ is the stage derivative. The input and output quantities at the beginning of step n are represented by $y^{[n-1]}$ and $y^{[n]}$, respectively.

Let $A = \{a_{ij}\}, B = \{b_{ij}\}, U = \{u_{ij}\}$ and $V = \{v_{ij}\}, \;\; 1 \leq i, j \leq n$ be the coefficient matrices, and $h \triangle x$ be the step size. The general form for a general linear method of order k is represented in matrix notation as

$$\begin{pmatrix} Y_i^{[n]} \\ y_i^{[n]} \end{pmatrix} = \left(\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right) \begin{pmatrix} hf(Y_i^{[n]}) \\ y_i^{[n-1]} \end{pmatrix}. \tag{1.2.5.4}$$

Chapter 2

Numerical Methods for Hamiltonian Systems

This chapter having the basic concepts for understanding the thesis work. This chapter is presents the structure-preserving numerical methods which keep the properties of a Hamiltonian system conserved. Classical numerical methods ignore the preservation of geometric properties. However, these properties are central to the study of a Hamiltonian system from the physical point of view. This apparent incompatibility of standard integrators for systems of ODEs naturally leads us to consider numerical methods which maintain the essential properties of Hamiltonian systems. Such numerical methods are known as structure-preserving or symplectic numerical methods.

The solutions of Hamiltonian systems possess invariants. The quadratic invariants of these systems are preserved by symplectic numerical methods which are especially constructed to this end. These methods accomplish the important task of preserving the first integrals of the Hamiltonian equations of motion. They are helpful in the long-term simulation of Hamiltonian systems and provide better mathematical results for diverse real-world problems.

The symplectic Euler method, a variation of the explicit Euler method, preserves the symplectic property for the flow of a Hamiltonian system. These methods preserve the geometry of the phase space Π of a Hamiltonian system. Hamiltonian systems are solved numerically using an approximation H_{approx} for the Hamiltonian energy function $H = H(p_1, ..., p_n; q_1, ..., q_n)$.

2.1 Differentiable Manifolds

Manifolds comprise an important subclass of topological spaces. They are frequently encountered in differential systems for idealized real-world problems. Manifolds are useful in that they generalize the geometric structure of finite-dimensional topological linear spaces which is useful for modelling physical systems. Many of the well-understood properties of the familiar Euclidean space $\mathbb{R}^n$ carry over naturally.

The class of topological manifolds is the most general class of manifolds. These are topological spaces with only manifold structure imposed on them. Depending upon the additional structure that they may have, there are various types of topological manifolds but we are only concerned with the subclass of differentiable manifolds.

Definition 2.1.1. *A topological space (M, τ) which is locally homeomorphic to a Euclidean space $\mathbb{R}^n$ for some $n \in \mathbb{N}$, is said to be a* ***topological manifold of dimension*** *n.*

Topological manifolds are the manifolds per se and the adjective topological is often omitted. The sphere $S_a^n = \{x \mid x \in \mathbb{R}^{n+1} \ \wedge \parallel x \parallel = a\}$ is a manifold of dimension n as it is locally homeomorphic to $\mathbb{R}^n$.

2.2 Quadratic Invariants

Consider the following autonomous initial-value problem in normal form

$$Dy = f(y), \ \ y(x_0) = y_0 \tag{2.2.0.1}$$

Suppose $Q(y) = yAy^*$ is a quadratic invariant, i.e. $DQ(y)f(y) = 0$, with A symmetric matrix of order n. It is an invariant of (2.2.0.1) if $y^T A f(y) = 0$.

2.3 Hamiltonian Systems

Hamiltonian mechanics is the formulation of classical mechanics by the Irish mathematician Sir William Rowan Hamilton (1805-1865). The **Hamiltonian equations of motion** for a classical mechanical system depend upon the generalized coordinates q_i and the generalized momenta p_i of the system, where the index $i = 1, ..., N$ and N is the degree of freedom for the system. If $p_i = p_i(x)$ and $q_i = q_i(x)$, then the Hamiltonian system of equations of motion for a system with N degrees of freedom are

$$\frac{dp_i}{dt} = -\partial_{q_i} H, \;\; \frac{dq_i}{dt} = \partial_{p_i} H, \;\; i = 1, ..., N. \tag{2.3.0.1}$$

Here $H = H(p_i; q_i) = H(p_1, ..., p_N; q_1, ..., q_N)$ represents the **total energy of the system** in consideration also known as its **Hamiltonian**. It is defined as the sum of the **kinetic energy** $K = K(p_i) = K(p_1, ..., p_N)$ and the **potential energy** $V = V(q_i) = V(q_1, ..., q_N)$ of the mechanical system

$$H(p_i; q_i) = K(p_i) + V(q_i). \tag{2.3.0.2}$$

2.4 Properties of Hamiltonian Systems

The Hamiltonian systems possess some special properties due to their intrinsic structure. These include **energy conservation property** and the **symplectic flow property**. In the following subsections, we explain the implications of these two important properties using example of a harmonic oscillator [1].

2.4.1 Energy Conservation Property

Total energy $H = H(p_i; q_i)$ of a Hamiltonian system is conserved. Mathematically, this is stated as

$$\frac{dH}{dt} = \sum_i \Big(\frac{\partial H}{\partial p_i} \frac{dp_i}{dt} + \frac{\partial H}{\partial q_i} \frac{dq_i}{dt} \Big) = \sum_i \Big(-\frac{\partial H}{\partial p_i} \frac{\partial H}{\partial q_i} + \frac{\partial H}{\partial q_i} \frac{\partial H}{\partial p_i} \Big) = 0. \tag{2.4.1.1}$$

Here the second equality is obtained using the Hamiltonian equations of motion given above.

Example 1. {*Energy Conservation in Harmonic Oscillator*}
Harmonic oscillator is a simple Hamiltonian system with only a single degree of freedom $N = 1$. In a standard normalized harmonic oscillator, a unit mass $m = 1$ is attached to a spring Σ with position coordinate $q_1 = q$ and momentum $p_1 = p$. Without loss of generality, we can choose our units of measurement such that the spring constant k of Σ is unity $k = 1$.

With these conventions, the kinetic energy and the potential energy of the harmonic oscillator are $K(p) = \frac{1}{2}\frac{p^2}{m} = \frac{1}{2}p^2$ and $V(q) = \frac{1}{2}kq^2 = \frac{1}{2}q^2$, respectively. By definition, the total energy $H(p, q)$ of the system is

$$H(p, q) = K(p) + V(q) = \frac{1}{2}(p^2 + q^2). \tag{2.4.1.2}$$

The Hamiltonian equations of motion for a harmonic oscillator are

$$\frac{dp}{dt} = -q, \quad \frac{dq}{dt} = p. \tag{2.4.1.3}$$

Using these equations of motion, it is easy to see that

$$\frac{dH}{dt} = \frac{\partial H}{\partial p}\frac{dp}{dt} + \frac{\partial H}{\partial q}\frac{dq}{dt} = -pq + qp = 0. \tag{2.4.1.4}$$

This shows that the Hamiltonian $H(p, q)$ of the system does not change with time and **the total energy of a harmonic oscillator is conserved**.

2.4.2 Symplectic Flow Property

The symplectic flow property is a useful property possessed by Hamiltonian mechanical systems. In this section we explain this property. We begin by giving the following definition.

Definition 2.4.1. *The phase space Π of a Hamiltonian system with generalized coordinates q_i and generalized momenta $p_i, i = 1, ..., N$ is the $2N$-dimensional real linear space generated by $\beta = \{p_1, ..., p_N, q_1, ..., q_N\}$ which is taken as its standard ordered basis. A point in Π is written $(p_1, ..., p_N; q_1, ..., q_N)$ using tuple notation or abbreviated as $(p_i; q_i)$.*

Next we define the symplecticity of a linear operator on the phase space of a Hamiltonian system.

Definition 2.4.2. *Let $T : \Pi \longrightarrow \Pi$ be a linear mapping on Π with (T) as its matrix of transformation. If J be the $2n \times 2n$ Jacobian matrix given by*

$$J = \left(\begin{array}{c|c} 0 & I_n \\ \hline -I_n & 0 \end{array}\right),$$

*the mapping T is said to be **symplectic** if $(T)^T J(T) = J$. The defining condition is referred to as **symplecticity condition**.*

Symplecticity of a linear mapping $T : \Pi \longrightarrow \Pi$ for the case $N = 1$ corresponds with the preservation of **oriented areas of parallelograms** represented by its transformation matrix (T). We conclude this section by defining the phase flow for a Hamiltonian system.

Definition 2.4.3. *Let ψ be the solution operator for a Hamiltonian system. The transformation of the phase space Π is a phase flow defined as*

$$\psi : (p_1(0), ..., p_N(0); q_1(0), ..., q_N(0)) \longmapsto (p_1(t), ..., p_N(t); q_1(t), ..., q_N(t)).$$

Example 2. {*Symplecticity of Harmonic Oscillator*} *Let ψ be the phase for a harmonic oscillator. We show that the phase flow $\partial\psi$ is a symplectic linear mapping on the phase space of this Hamiltonian system by using the symplecticity condition. Consider*

$$\psi = \begin{pmatrix} -q \\ p \end{pmatrix}, \quad \partial\psi = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

We now show that the flow of harmonic oscillator is symplectic using these values.

$$\partial\psi^T J \partial\psi = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = J.$$

2.4.3 Simple Harmonic Oscillator

Consider a simple harmonic oscillator with $y = (p, q)^*$. Using the Hamiltonian equations of motion $\dot{p} = -q, \ \ \dot{q} = p$ for this system, we have

$$f(y) = \dot{y} = (-q, p)^*. \tag{2.4.3.1}$$

Let us take $Q(y) = yAy^*$ with $A = \frac{1}{2}I_2$ and check $Q(y)$ for quadratic invariance. This is done by using the invariance condition $yQ(y)f(y) = 0$ which is satisfied as

$$yQ(y)f(y) = (p, q) \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} (-q, p)^* = 0.$$

Hence, $Q(y)$ is a quadratic invariant of the differential system of a simple harmonic oscillator.

The explicit Euler method is

$$\begin{aligned} p_{n+1} &= p_n + hf(q_n) = p_n - hq_n, \\ q_{n+1} &= q_n + hf(p_n) = q_n + hp_n, \end{aligned} \tag{2.4.3.2}$$

and

$$\psi = (p_n - hq_n, q_n + hp_n), \;\; D\psi = \begin{pmatrix} 1 & -h \\ h & 1 \end{pmatrix}. \tag{2.4.3.3}$$

We check for the symplecticity of this system using explicit Euler method

$$D\psi^* J D\psi = \begin{pmatrix} 0 & h^2 + 1 \\ -(h^2 + 1) & 0 \end{pmatrix} \neq J$$

with

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

This shows that the explicit Euler method does not preserve the symplectic property for the phase flow ψ of this Hamiltonian system.

2.5 Symplectic Euler Mthod

The symplectic Euler method is a modification of the explicit Euler method. It yields better results as compared to the explicit Euler method. The symplectic Euler method is applied to a pair of ordinary differential equations

of the form

$$\dot{y} = f(x, y), \;\; \dot{v} = g(x, v)$$

with $f(x, y)$ and $g(x, v)$ as the defining functions for the equations. If the Hamiltonian H is written $H = K + V$, the equations of motion for a simple harmonic oscillator

$$\dot{p} = -q, \;\; \dot{q} = p$$

are solved with the initial condition $(p_0, q_0) = (1, 0)$. The general form of the symplectic Euler method is

$$\begin{aligned} v_{n+1} &= v_n + g(x_n, y_n) \triangle x \\ y_{n+1} &= y_n + f(x_n, v_{n+1}) \triangle x \end{aligned}$$

Here $\triangle x$ is the time step and $x_n = x_0 + n\triangle x$ is the time elapsed after n steps. The symplectic Euler method uses v_{n+1} in the equation in place of x_{n+1}, while the Euler method uses v_n. Symplectic Euler method preserves the symplecticity of the Hamiltonian system, hence the name. This is proved by using the symplecticity condition $\psi' J \psi = J$. Here J is a symmetric matrix with determinant 1.

Example 3. *The motion of a spring satisfying Hooke's law is given by*

$$\frac{dx}{dt} = v(t), \;\; \frac{dv}{dt} = -\omega^2 x. \tag{2.5.0.1}$$

Applying symplectic Euler method to the system gives

$$\begin{aligned} v_{n+1} &= v_n - \omega^2 x_n \triangle t \\ x_{n+1} &= x_n - (v_n - \omega^2 x_n \triangle t) \triangle t. \end{aligned}$$

The sysmplectic Euler method preserves the symplectic property of the system, as

$$D\psi = \begin{pmatrix} 1 & -\omega^2 \triangle t \\ \triangle t & 1 - \omega^2 \triangle^2 t \end{pmatrix}$$

$$D\psi^* J D\psi = \begin{pmatrix} 1 & -\omega^2 \triangle t \\ \triangle t & 1 - \omega^2 \triangle^2 t \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 1 & -\omega^2 \triangle t \\ \triangle t & 1 - \omega^2 \triangle^2 t \end{pmatrix} = J.$$

2.5.1 Perturbed Kepler Problem

The Kepler problem is a special case of the two-body problem in which the two bodies interact by a central force F that varies in strength as the inverse square of the distance r between them. Equations of motion for the perturbed Kepler problem are, [7].

$$\begin{aligned} Dq_1 &= p_1, \\ Dq_2 &= p_2, \\ Dp_1 &= -\frac{q_1}{\sqrt{({q_1}^2+{q_2}^2)^3}} - \frac{0.0075q_1}{\sqrt{({q_1}^2+{q_2}^2)^3}} \\ Dp_1 &= -\frac{q_2}{\sqrt{({q_1}^2+{q_2}^2)^3}} - \frac{0.0075q_2}{\sqrt{({q_1}^2+{q_2}^2)^3}} \end{aligned}$$

where (q_1, q_2) and (p_1, p_2) are the generalized coordinates and generalized momenta respectively. The Hamiltonian of the system is

$$H(p_1, p_2; q_1, q_2) = \frac{1}{2}({p_1}^2 + {p_2}^2) - \frac{1}{\sqrt{({q_1}^2+{q_2}^2)}} - \frac{0.005}{2\sqrt{({q_1}^2+{q_2}^2)^3}}$$

The initial conditions are

$$(q_1, q_2) = (1-e, 0), \;\; (p_1, p_2) = (0, \sqrt{1+e}/\sqrt{1-e}).$$

For this problem we know two first integrals: the Hamiltonian function $H(p, q)$ and the angular momentum $L(p, q) = q_1p_2 - q_2p_1$. In this experiment we observed the conservation of energy for perturbed Kepler problem with step-size $h = 0.01$ and eccentricity $e = 0$. The energy error is calculated by subtracting the energy calculated at initial value given with the perturbed Kepler problem from the energy calculated at approximated value, i.e. energy error$= H_{\approx} - H$.

The error in energy is shown in the Figures below. Here we used symplectic Euler method to bound the energy error of perturbed Kepler problem.

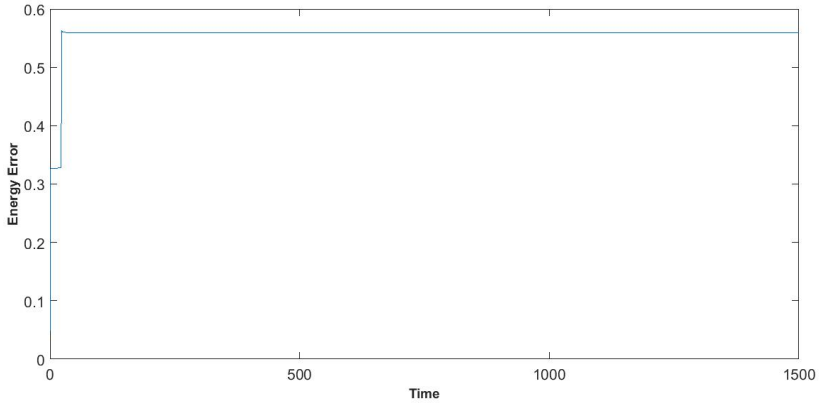

Figure 2.1: Energy error of the perturbed Kepler problem using Euler method.

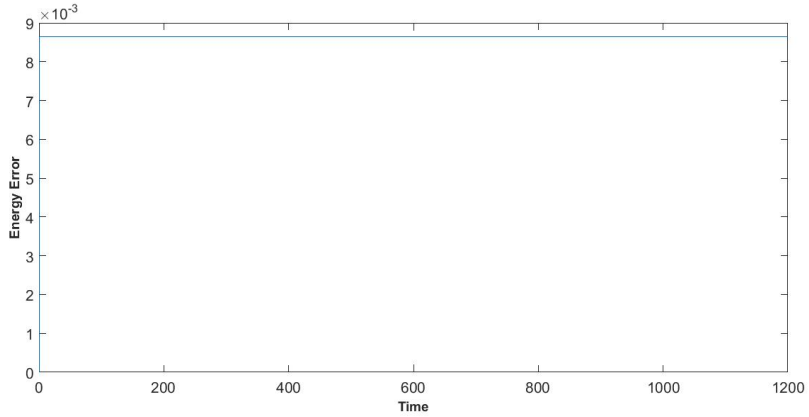

Figure 2.2: Symplectic Euler method applied to the perturbed Kepler problem.

We observed that the Hamiltonian of the system is not bounded when Explicit Euler method is used with step size h = 0.01. Geometric properties of the Hamiltonian system does not remains preserved with Explicit Euler method. In next experiment we used symplectic Euler method which gives great preservation of quadratic invariants and the absolute error of the energy remains bounded under this method.

2.6 Symplectic Runge-Kutta Methods

A Runge-Kutta method is symplectic if the numerical solution y_n has $Q(y_n)$ as the quadratic invariant and the condition

$$< y_n, y_n >=< y_{n-1}, y_{n-1} >$$

holds. A method has this property if and only if,

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0 \qquad forall \quad i, j.$$

Solutions of the Hamiltonian systems possess the characteristic property named as Symplecticness. Symplectic Runge-Kutta methods, when applied to Hamiltonian system, inherit this property along with numerical solution.

Proof:

Generally Runge-Kutta method is defined as,

$$\begin{aligned} Y_i &= y_{n-1} + h\sum_{j=1}^{s} a_{ij} f(Y_j), \qquad i, j = 1, 2, ..., s, \\ y_n &= y_{n-1} + h\sum_{i=1}^{s} b_i f(Y_i). \end{aligned} \tag{2.6.0.1}$$

Consider an initial value problem;

$$y'(x) = f(y(x)), \qquad y(x_0) = y_0$$

Now we apply the condition of symplecticity taking C as a symmetric matrix. The condition $b_i b_j - b_i a_{ij} - b_j a_{ji}$ with the assumption $y^T C f(y) = 0$

states that

$$y_1{}^T C y_1 = y_0{}^T C y_0$$

or

$$< y_1, y_1 >=< y_0, y_0 >$$

The above condition shows that the method is symplectic if,

$$(b_i b_j - b_i a_{ij} - b_j a_{ji}) Y_i^T C Y_j = 0$$

The system is explicit if $a_{ij} = 0$ for $j = i$. The condition for such a method to be symplectic is

$$(b_i b_j - b_i a_{ij} - b_j a_{ji}) = 0$$

This condition implies that Runge Kutta methods are necessarily implicit.

2.6.1 Harmonic Oscillator

We solve harmonic oscillator equations

$$p' = -q, \qquad q' = p$$

with $h = 0.01$ and $p_0 = 1$, $q_0 = 0$ and the Hamiltonian of the system is

$$H = \frac{p^2}{2} + \frac{q^2}{2}$$

using an explicit RK method given as and using an implicit Runge-Kutta method given as

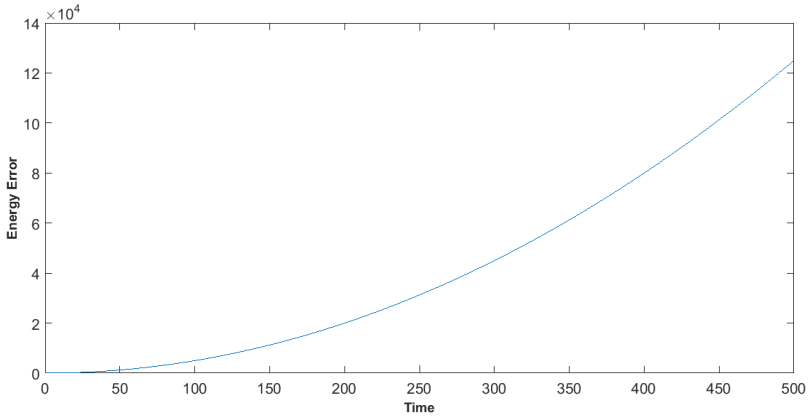

Figure 2.3: The energy error of a Harmonic oscillator by Explicit Runge-Kutta method

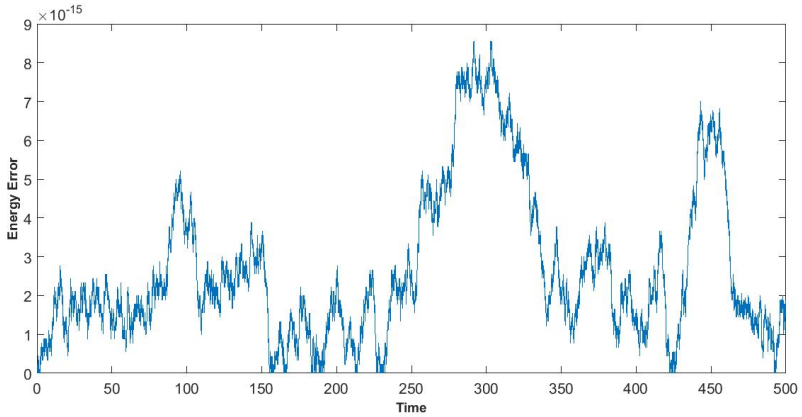

Figure 2.4: The energy error of a Harmonic oscillator by Symplectic Runge-Kutta method

Figure 2.3 and Figure 2.4 show that the symplectic (implicit) Runge-Kutta method can preserve the geometric properties of the Hamiltonian system. Energy error is also remains bounded over the time interval whereas the explicit Runge-Kutta method cannot preserve energy.

2.7 $G-$Symplectic General Linear Methods

General linear methods are a unified class of conventional numerical methods used to solve Hamiltonian systems numerically. Despite their usefulness, these methods do not preserve the phase flow ψ of the system. Because of their multi-step and muti-value nature, these methods cannot achieve true conservation of the quadratic invariants of a Hamiltonian system. Quadratic invariants and symplecticity are preserved by one-step methods. Only G-symplectic GLM can preserve quadratic invariant.

A Hamiltonian system also known as conservative problem, having the property,

$$< y, f(y) >= 0$$

can be solved by general linear method but we require

$$< y^{[n]}, y^{[n]} >_G = < y^{[n-1]}, y^{[n-1]} >_G$$

Symplectic condition for one-step methods parallels this condition but for r input vectors and output vectors and G is a symmetric matrix of order $r \times r$.

G-symplectic general linear methods are constructed to preserve the symplectic invariants of a Hamiltonian system. These methods also preserve the total energy and the symplectic invariants of the system over extended periods of time. They possess properties similar to the symplectic Runge-Kutta methods.

Theorem 1. *A general linear method is said to be G-symplectic, if there exist a diagonal $s \times s$ matrix D and a symmetric $r \times r$ matrix G such that*

$$\begin{aligned} V^T G V &= G, \\ DU &= B^T G V, \\ DA + A^T D &= B^T G B. \end{aligned}$$

are satisfied.

General linear methods cannot be symplectic because these methods cannot preserve true quadratic invariants. However, G-symplectic general linear methods under a G-norm, preserve the quadratic behavior of invariants.

Example 4. *Consider the implicit fourth-order GLMs with two stages and two output values having coefficient matrix*

$$\left(\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right) = \left(\begin{array}{cc|cc} \frac{3+\sqrt{3}}{6} & 0 & 1 & -\frac{3+2\sqrt{3}}{3} \\ -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 & \frac{3+2\sqrt{3}}{3} \\ \hline \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & -1 \end{array}\right) \tag{2.7.0.1}$$

The matrix A is a lower triangular matrix. The general representation of this method is given below;

$$\begin{aligned} {Y_1}^{[n]} &= h(\frac{3+\sqrt{3}}{6}) f({Y_1}^{[n]}) + {y_1}^{[n-1]} - (\frac{3+2\sqrt{3}}{3}) {y_2}^{[n-1]} \\ {Y_2}^{[n]} &= -h(\frac{\sqrt{3}}{3}) f({Y_1}^{[n]}) + h(\frac{3+\sqrt{3}}{6}) f({Y_2}^{[n]}) + {y_1}^{[n-1]} + (\frac{3+2\sqrt{3}}{3}) {y_2}^{[n-1]} \\ {y_1}^{[n]} &= (\frac{h}{2}) f({Y_1}^{[n]}) + (\frac{h}{2}) f({Y_2}^{[n]}) + {y_1}^{[n-1]} \\ {y_2}^{[n]} &= (\frac{h}{2}) f({Y_1}^{[n]}) - (\frac{h}{2}) f({Y_2}^{[n]}) - {y_2}^{[n-1]} \end{aligned} \tag{2.7.0.2}$$

This general linear method is G-symplectic if the conditions of the theorem are satisfies with matrices G and D. Consider the matrices G and D as;

$$G = \begin{pmatrix} 1 & g_{12} \\ g_{21} & g_{22} \end{pmatrix}, \qquad D = \begin{pmatrix} d_{11} & 0 \\ 0 & d_{22} \end{pmatrix}$$

We obtain the following values for the entries of the matrix D

$$\begin{aligned} d_{11} &= \frac{b_{11} + b_{21}v_{21} - b_{11}v_{22}}{1 - v_{22}} = \frac{1}{2} \\ d_{22} &= \frac{b_{12} + b_{22}v_{12} - b_{12}v_{22}}{1 - v_{22}} = \frac{1}{2} \end{aligned}$$

Similarly for matrix G we consider the first and third conditions of Theorem (2.1.1), we obtain

$$\begin{aligned} g_{12} &= \frac{v_{12}}{1 - v_{22}} = 0 \\ g_{21} &= \frac{d_{11} - b_{11}g_{11}}{b_{21}} = 0 \\ g_{22} &= \frac{d_{22}u_{22}}{b_{22}v_{22}} = \frac{3 + 2\sqrt{3}}{3} \end{aligned}$$

So the matrices G and D becomes;

$$G = \begin{pmatrix} 1 & 0 \\ 0 & \frac{3+2\sqrt{3}}{3} \end{pmatrix}, \qquad D = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}$$

since

$$\begin{aligned} A &= \begin{pmatrix} \frac{3+\sqrt{3}}{6} & 0 \\ -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} \end{pmatrix}, \qquad B = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{pmatrix} \\ U &= \begin{pmatrix} 1 & -\frac{3+2\sqrt{3}}{3} \\ 1 & \frac{3+2\sqrt{3}}{3} \end{pmatrix}, \qquad V = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{aligned}$$

This method should satisfy the given conditions:

$$\begin{aligned} V^T GV &= G, \\ B^T GV &= DU, \\ B^T GB &= DA + A^T DDA + A^T D. \end{aligned}$$

Now we prove that each condition is satisfied separately.

$$\begin{aligned} V^TGV &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}^T \begin{pmatrix} 1 & 0 \\ 0 & \frac{3+2\sqrt{3}}{3} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -\frac{3+2\sqrt{3}}{3} \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \\ 0 & \frac{3+2\sqrt{3}}{3} \end{pmatrix} \\ &= G. \end{aligned}$$

So first condition is satisfied.

Now consider

$$\begin{aligned} DU &= \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 1 & -\frac{3+2\sqrt{3}}{3} \\ 1 & \frac{3+2\sqrt{3}}{3} \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{2} & -\frac{3+2\sqrt{3}}{6} \\ \frac{1}{2} & \frac{3+2\sqrt{3}}{6} \end{pmatrix} \end{aligned}$$

and

$$\begin{aligned} B^TGV &= \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{pmatrix}^T \begin{pmatrix} 1 & 0 \\ 0 & \frac{3+2\sqrt{3}}{3} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{2} & -\frac{3+2\sqrt{3}}{6} \\ \frac{1}{2} & \frac{3+2\sqrt{3}}{6} \end{pmatrix} \\ &= DU \end{aligned}$$

which satisfies the second condition $DU = B^TGV$.

Now considering,

$$\begin{aligned} B^TGB &= \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{pmatrix}^T \begin{pmatrix} 1 & 0 \\ 0 & \frac{3+2\sqrt{3}}{3} \end{pmatrix} \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{pmatrix} \\ &= \begin{pmatrix} \frac{3+\sqrt{3}}{6} & \frac{\sqrt{3}}{6} \\ \frac{\sqrt{3}}{6} & \frac{3+\sqrt{3}}{6} \end{pmatrix} \end{aligned}$$

and

$$\begin{aligned} DA + A^T D &= \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \frac{3+\sqrt{3}}{6} & 0 \\ -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} \end{pmatrix} + \begin{pmatrix} \frac{3+\sqrt{3}}{6} & 0 \\ -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} \end{pmatrix}^T \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \\ &= \begin{pmatrix} \frac{3+\sqrt{3}}{6} & \frac{\sqrt{3}}{6} \\ \frac{\sqrt{3}}{6} & \frac{3+\sqrt{3}}{6} \end{pmatrix} \\ &= B^T G B \end{aligned}$$

2.7.1 Simple Pendulum

Consider the simple pendulum with equations of motion,

$$\begin{aligned} q' &= p, \\ p' &= -sin(q) \end{aligned}$$

where the Hamiltonian of the system is

$$H = \frac{p^2}{2} - cos(q)$$

G-sympletic general linear methods have been applied to solve simple pendulum with the initial conditions $q = 2.3, p = 0$. Energy error is plotted in the Figure given below for 10000 steps with step-size $h = 0.01$.

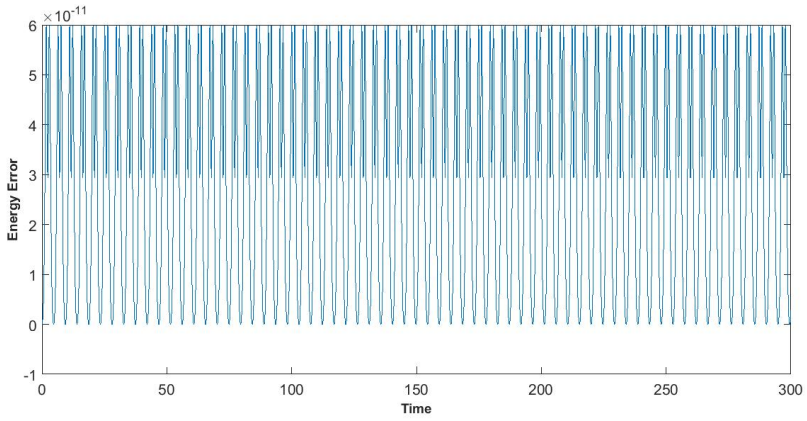

Figure 2.5: Energy conservation of the simple pendulum problem by using G-symplectic GLM's with initial value $p = 0$ and $q = 2.3$

This graph is plotted between time along x-axis and the energy error H_{err} along y-axis.

The use of G-symplectic general linear method gives values of H_{err} closer to 0 with the additional benefit that the Hamiltonian (energy) of the system is always conserved.

Chapter 3

General Linear Methods with Projection

3.1 Projection Technique

Consider an autonomous initial value problem

$$Dy = f(y), \;\; y(x_0) = y_0. \tag{3.1.0.1}$$

The solution space of this initial value problem is a smooth manifold.

$$M = \{y; \quad g(y) = 0\}, \tag{3.1.0.2}$$

where $g : \mathbb{R}^n \to \mathbb{R}^m$ and the differential equation satisfying the property that

$$y_0 \; \epsilon \; M \;\; \Rightarrow \;\; y(t)\epsilon M, \quad \forall t \tag{3.1.0.3}$$

The equation given 3.1.0.3 is equal to $g'(y)f(y) = 0$ for $y \;\; \in \;\; M$. However we require $g'(y)f(y) = 0$ for the conservation of invariants for all $y \in \mathbb{R}^n$. Therefore, $y' = f(y(t))$, represents a differential equation on the manifold M and $g(y)$ is an invariant.

Numerical methods which avoid the use of local coordinates, can be divided into a) methods for which the numerical solution automatically stays on M without using explicitly the function $g(y)$, and b) methods which, after every successful step, project the numerical approximation onto the manifold M. To the first class belong symplectic one-step methods, if $g(y) = y^T Cy$ is a quadratic first integral (i.e., $g'(y)f(y) = 0$ for all y in a neighborhood of the solution).

Hamiltonian system has invariants, and these invariants can be conserved automatically by using certain numerical methods. In other words, when numerical method fails to conserve the geometric properties of the given Hamiltonian system of the differential equation then we apply projection method to project the numerical solution of the Hamiltonian system onto

the invariant manifold. We remove the integral error by projecting the solution on the integral manifold. This is the main idea behind this method.

Our interest lies in those numerical methods with which we can minimize the error and conserve the invariants of the systems. The first approach is to use only on $G-$symplectic general linear method to preserve the invariants related to Hamiltonian system. Secondly, we can use projection technique with one-step methods to conserve the systems. Here we applied different methods to the different systems and observed the results. We solve some Hamiltonian systems by applying Euler method, symplectic Euler method, GLMs, and G-symplectic GLMs with projection technique to conserve the geometric properties of these systems.

3.2 Standard Projection Technique

Projection technique is an approach to the numerical solution of differential equations on manifolds. The starting algorithm for a standard projection method is to first apply a numerical method taking the initial value y_n to $\tilde{y}_{n+1}$ and then get y_{n+1} by projecting it back onto the invariant manifold $M = \{y \mid g(y) = 0\}$ of the system.

The algorithm for a single step of projecting the numerical solution onto the integral manifold is [7].

- Use initial condition $y(x_0) = y_0$ and apply a general linear method to get $\tilde{y}_1^{[1]}$.
- Project the value of first component of general linear methods to the manifold as

$$y_1{}^{[1]} = \tilde{y}_1^{[1]} + \nabla H(y_1{}^{[1]}) \times \frac{H(y_0) - H(\tilde{y}_1^{[1]})}{\nabla H(\tilde{y}_1^{[1]}).\nabla H(\tilde{y}_1^{[1]})} \tag{3.2.0.1}$$

Let

$$\lambda = \frac{H(y_0) - H(\tilde{y}_1^{[1]})}{\nabla H(\tilde{y}_1^{[1]}).\nabla H(\tilde{y}_1^{[1]})}$$

$H(y_0)$ and $\nabla H(y)$ denote the initial value of $H(y)$ and its Jacobian, respectively. The projection is applied only on first output value ${y_1}^{[1]}$. The equation (3.2.0.1) is implicit, hence Newton iterations are used to solve this equation for ${y_1}^{[1]}$. Using these conventions, (3.2.0.1) becomes

$${y_1}^{[1]} - \tilde{y_1}^{[1]} - \nabla H({y_1}^{[1]})\lambda = 0, \;\; g({y_1}^{[1]}) = 0. \tag{3.2.0.2}$$

We replace ${y_1}^{[1]}$ with $\tilde{y_1}^{[1]}$ in $\nabla H({y_1}^{[1]})$. The following stopping criteria is used in Newton iteration method

$$\| \; {y_1}^{[1]} - \tilde{y_1}^{[1]} \| < TOL = 10^{-15}. \tag{3.2.0.3}$$

Standard projection method gives excellent results in conserving the invariants of Hamiltonian systems. The projection is applied at the end of each of the integration step.

3.2.1 Simple Pendulum

The Hamiltonian equations of motion defining the simple pendulum with the generalized momentum $p(x)$ and the generalized coordinate $q(x)$ are

$$\dot{p} = -sinq, \;\; \dot{q} = p. \tag{3.2.1.1}$$

The total energy $H(p, q)$ of the system is

$$H = \frac{p^2}{2} - cosq. \tag{3.2.1.2}$$

This is an invariant for the Hamiltonian system of a simple pendulum. We apply explicit Euler method to the Hamiltonian system with initial conditions $p = 1$, $q = 0$, and step size $h = 0.01$. Energy error is calculated

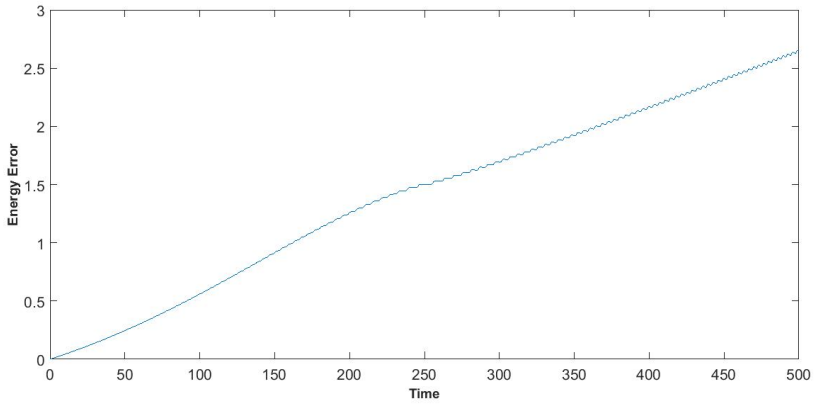

Figure 3.1: Energy conservation of a simple pendulum using explicit Euler method with initial condition $(p_0, q_0) = (1, 0)$ and step size $h = \triangle x = \frac{1}{100}$.

by subtracting the approximated energy from the its actual value. We observe that Euler method does not preserve the Hamiltonian of the system as shown in Figure 3.1. Next we apply the projection technique with Euler method and observe the results. It projects the numerical solution of the system onto the invariant manifold M to keep the total energy $H = H(p, q)$ of the system constant at each iteration. Invariants of a system remain conserved over longer intervals of time if the Euler method with projection technique is applied as shown in Figure 3.2.

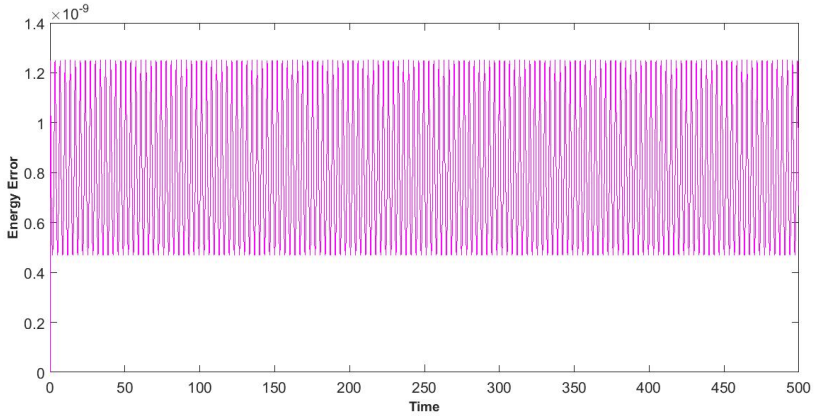

Figure 3.2: Energy conservation of a simple pendulum using explicit Euler method with projection technique with initial condition $(p_0, q_0) = (1, 0)$ and step size $h = \triangle x = \frac{1}{100}$.

It can be seen in Figure 3.3 that for the G-symplectic general linear methods (GLMs), simple pendulum shows good behavior. Energy of the systems remains conserved after applying G-symplectic general linear methods. Similarly when we apply projection technique along with this method it also gives good preservation of invariants of the system as shown in Figure 3.4.

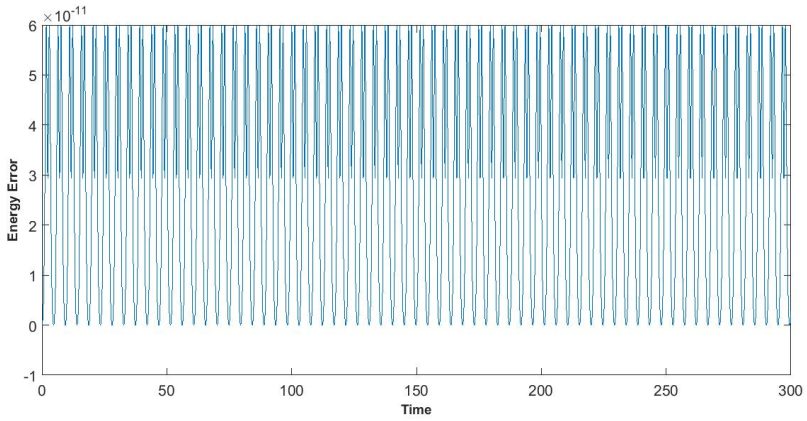

Figure 3.3: Energy conservation of a simple pendulum using G-symplectic GLMs without projection technique with initial condition $(p_0, q_0) = (1, 0)$ and step size $h = \triangle x = \frac{1}{100}$.

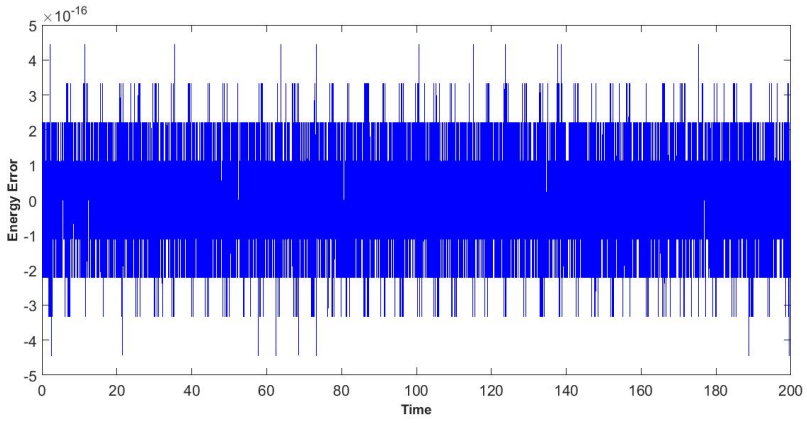

Figure 3.4: Energy conservation of a simple pendulum using G-symplectic GLMs with projection technique with initial condition $(p_0, q_0) = (1, 0)$ and step size $h = \triangle x = \frac{1}{100}$.

3.2.2 Simple Harmonic Oscillator

The equations of motion of simple harmonic oscillator

$$\frac{dp}{dx} = -q, \quad \frac{dq}{dx} = p. \tag{3.2.2.1}$$

The total energy of the system is

$$H(p, q) = \frac{p^2}{2} + \frac{q^2}{2}. \tag{3.2.2.2}$$

We apply explicit Euler method to harmonic oscillator with initial conditions $p = 1$, $q = 0$, and step size $h = 0.01$. We examine that Euler method does not preserve the total energy of the system as shown in Figure 3.5. When we apply the projection technique with Euler method, it keeps the total energy $H = H(p, q)$ of the system constant at each iteration as shown in Figure 3.6.

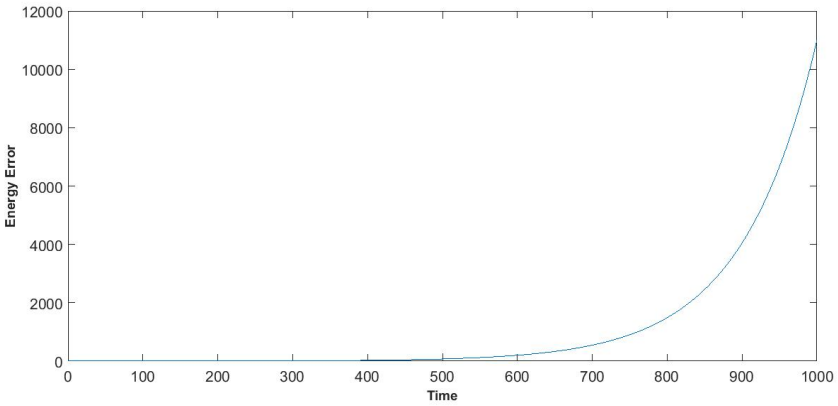

Figure 3.5: Euler method applied to the harmonic oscillator problem with initial condition $(p_0, q_0) = (1, 0)$ and step size $h = \triangle x = \frac{1}{100}$.

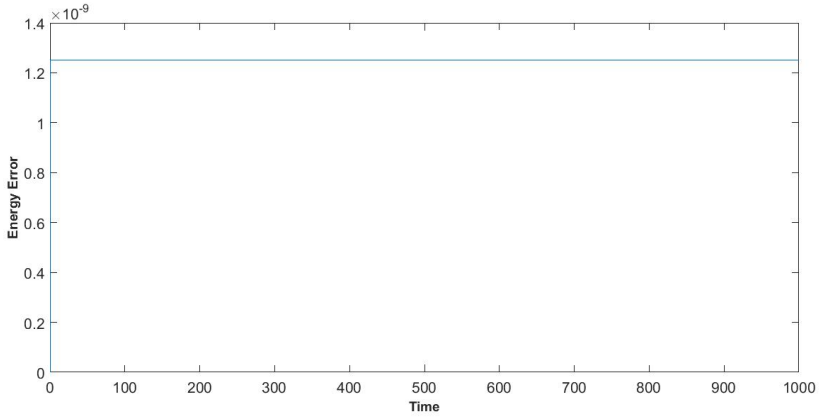

Figure 3.6: Euler method applied to the harmonic oscillator problem with projection technique with initial condition $(p_0, q_0) = (1, 0)$ and step size $h = \triangle x = \frac{1}{100}$.

Similarly, Runge-Kutta methods

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 1/3 & 1/3 & 0 & 0 & 0 \\ 2/3 & -1/3 & 1 & 0 & 0 \\ 1 & 1 & -1 & 1 & 0 \\ \hline & 1/8 & 3/8 & 3/8 & 1/8 \end{array}$$

without projection are applied to this Hamiltonian system with initial condition $(p_0, q_0) = (1, 0)$ and step size $h = \triangle x = \frac{1}{100}$ for $50,000$ steps and the energy error $\triangle H = H_{approx} - H$ is calculated, the results of the experiment are shown in the figure 3.7. Here time x is taken along x-axis and the energy error $\triangle H$ is plotted along y-axis.

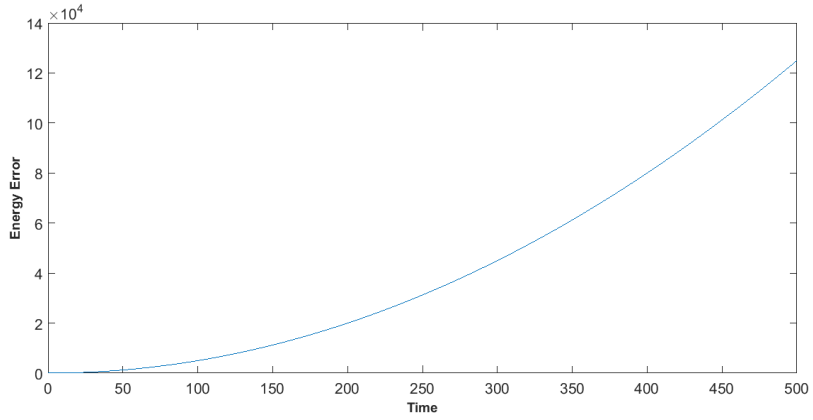

Figure 3.7: Explicit Runge-Kutta method applied to the harmonic oscillator problem with initial condition $(p_0, q_0) = (1, 0)$ and step size $h = \triangle x = \frac{1}{100}$.

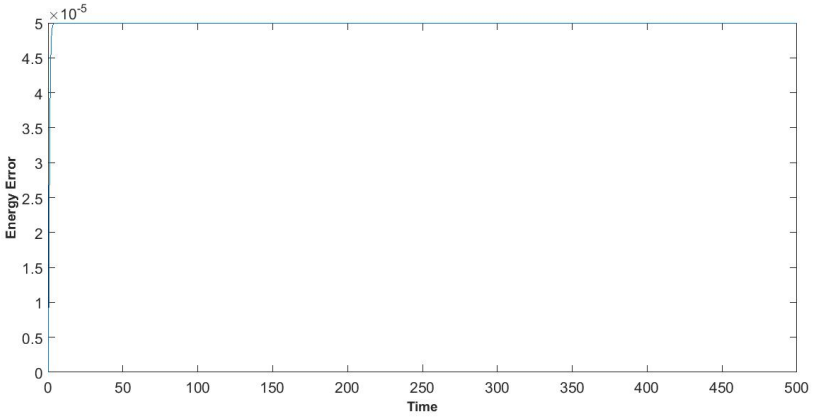

Figure 3.8: Explicit Runge-Kutta method with projection is applied to a harmonic oscillator problem with initial condition $(p_0, q_0) = (1, 0)$ and step size $h = \triangle x = \frac{1}{100}$.

This experiment shows that the error in the total energy is not bounded if explicit Runge-Kutta method is applied. However, when Runge-Kutta method is used with projection, it conserves the Hamiltonian $H(p, q)$ of the system by projecting the numerical solution onto the invariant manifold M at each iteration as shown in Figure 3.8.

We also apply symplectic Runge-Kutta method with and without projection technique to the harmonic oscillator. Results shows that the energy(hamiltonian) of harmonic oscillator remains constant over long time interval as given in Figure 3.9 and Figure 3.10.

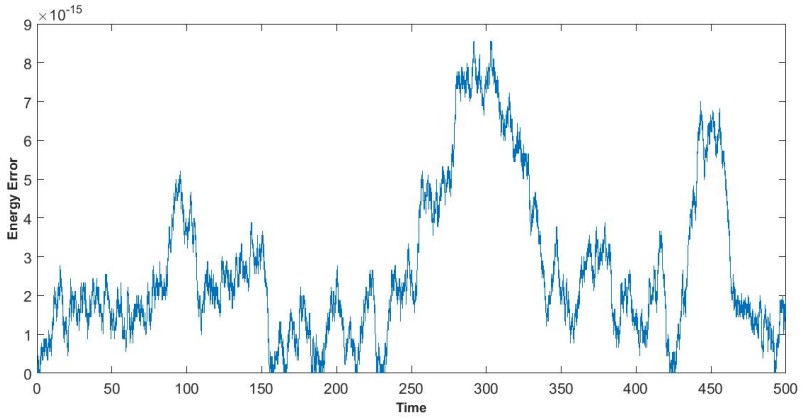

Figure 3.9: Symplectic Runge-Kutta method applied to the harmonic oscillator problem with initial condition $(p_0, q_0) = (1, 0)$ and step size $h = \triangle x = \frac{1}{100}$.

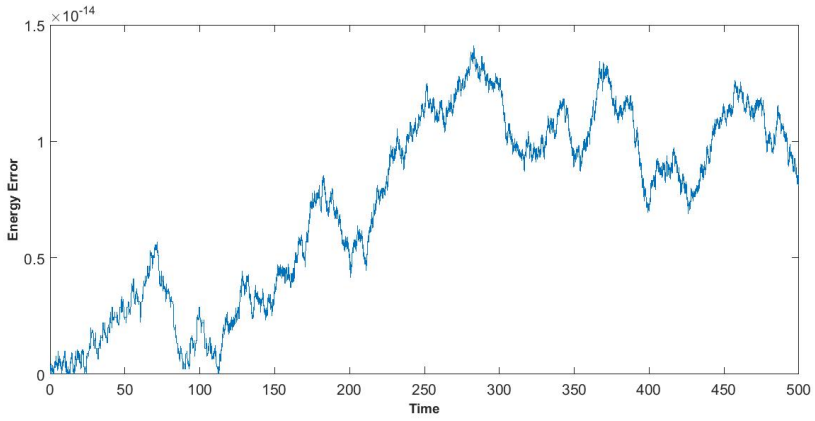

Figure 3.10: Symplectic Runge-Kutta method with projection technique is applied to the harmonic oscillator problem with initial condition $(p_0, q_0) = (1, 0)$ and step size $h = \triangle x = \frac{1}{100}$.

3.2.3 Perturbed Kepler Problem

The Hamiltonian $H = H(p_1, p_2, q_1, q_2)$ of the system is

$$H = \frac{1}{2}({p_1}^2 + {p_2}^2) - \frac{1}{\sqrt{({p_1}^2 + {p_2}^2)}} - \frac{0.005}{2\sqrt{({p_1}^2 + {p_2}^2)^3}} \qquad (3.2.3.0)$$

The initial conditions are

$$(q_1, q_2) = (1 - e, 0), \;\; (p_1, p_2) = (0, \sqrt{1+e}/\sqrt{1-e}). \qquad (3.2.3.0)$$

For this problem we know the two first integrals: the Hamiltonian function $H(p_1, p_2, q_1, q_2)$ and the angular momentum $L(p_1, p_2, q_1, q_2) = q_1 p_2 - q_2 p_1$. energy error is defined as the difference $\triangle H = H_{\approx} - H$ of the actual value for total energy H from its approximated value $H_{\approx}$.

We use to apply explicit Euler method and the symplectic Euler method with constant step size $h = \triangle x = \frac{3}{100}$. The results are shown in Figure 3.11 and Figure 3.12. The numerical solution obtained by using the explicit Euler method is unacceptable. The projection onto the invariant manifold improves the numerical solution, but it still has a wrong qualitative behavior. Only projection onto both invariants, $H(p, q) =$ Const and

$L(p, q) = Const$ gives the correct behavior.

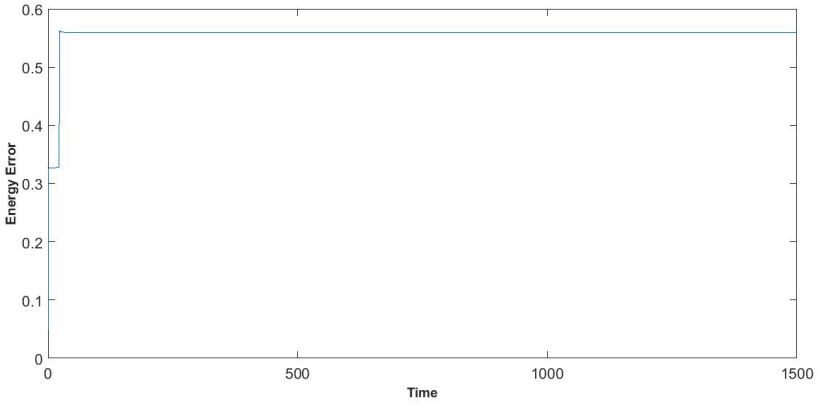

Figure 3.11: Results of the explicit Euler method without projection as applied to the perturbed Kepler problem with step size $\triangle x = \frac{3}{100}$.

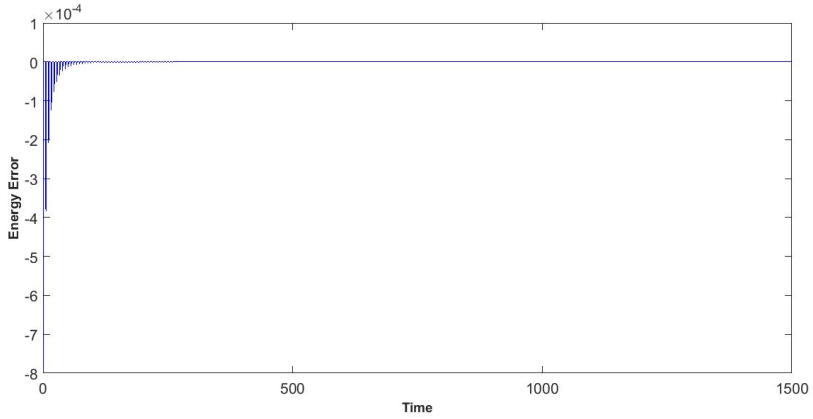

Figure 3.12: Energy error of perturbed Kepler problem using explicit Euler method with projection of H with step size $\triangle x = \frac{3}{100}$.

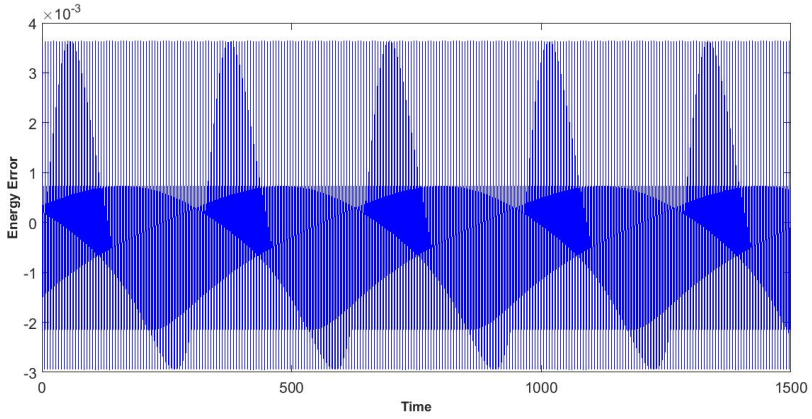

Figure 3.13: Results of explicit Euler method with projection of both H and L invariants of perturbed Kepler problem with step size $\triangle x = \frac{3}{100}$.

The symplectic Runge-Kutta method shows the correct behavior without any projection. A projection onto $M_H = \{p_1, p_2, q_1, q_2 \mid H(p_1, p_2, q_1, q_2) = c\}$ alone destroys this behavior while the projection onto both the invariant manifolds M_H and M_L corrects this anomaly as shown in Figure 3.14, Figure 3.15 and Figure 3.16.

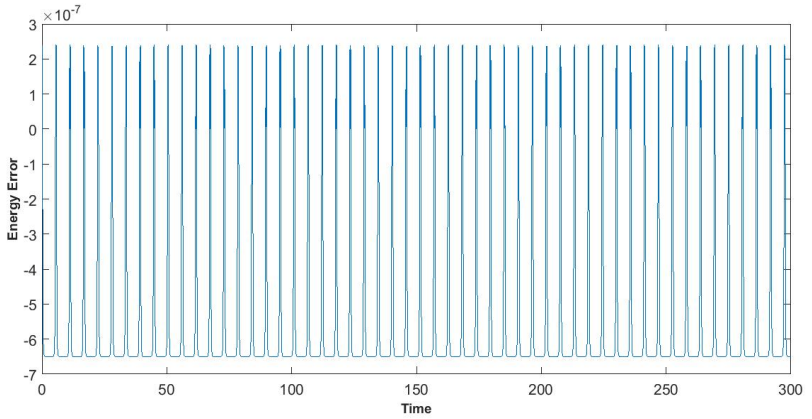

Figure 3.14: Results of the symplectic Runge-Kutta method without projection as applied to the perturbed Kepler problem with step size $\triangle x = \frac{3}{100}$.

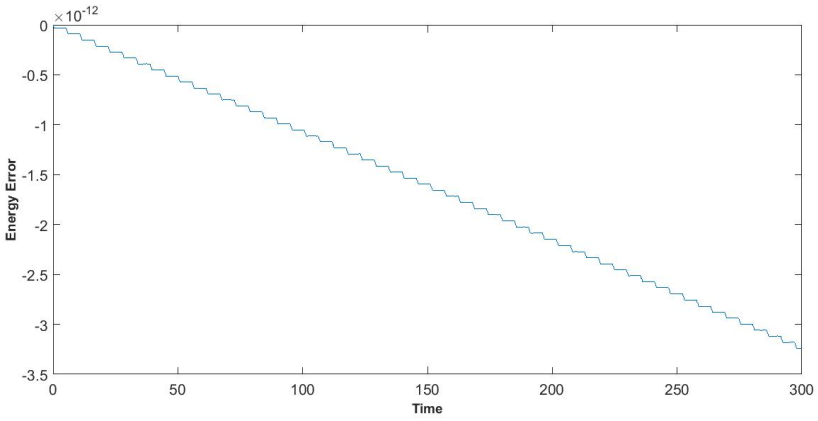

Figure 3.15: Symplectic Runge-Kutta method applied onto M_H alone with projection to the perturbed Kepler problem with step size $\triangle x = \frac{3}{100}$.

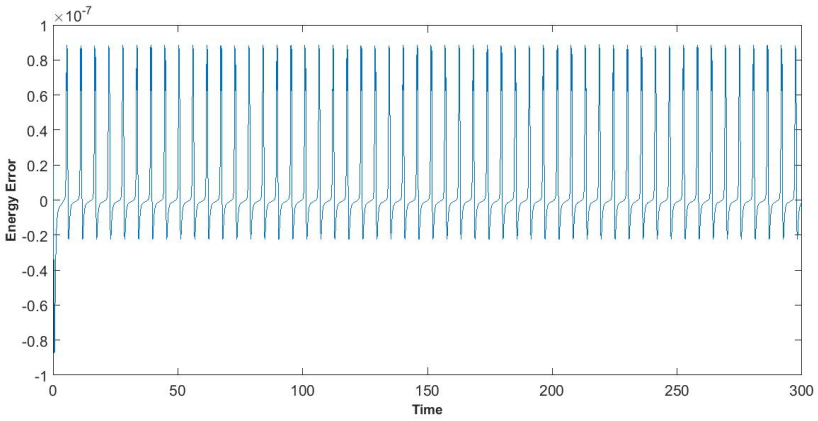

Figure 3.16: Symplectic Runge-Kutta method with projection is applied onto both M_H and M_L invariants of perturbed Kepler problem with step size $\triangle x = \frac{3}{100}$.

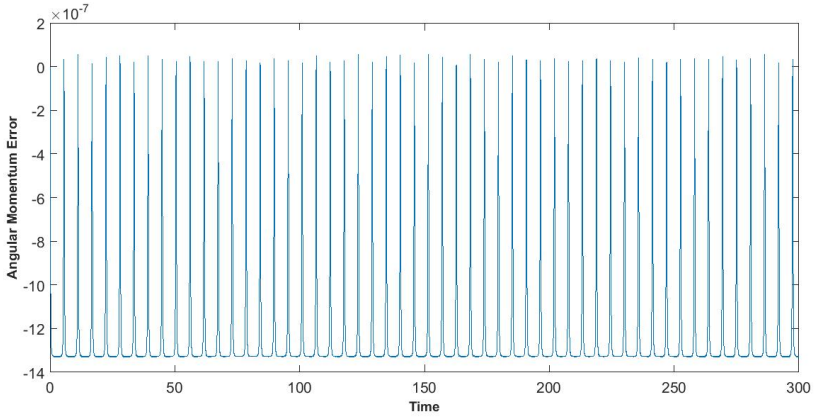

Figure 3.17: Energy error of perturbed Kepler problem using $G-$symplectic GLM43 without projection

We apply fourth order $G-$symplectic GLMs,

$$\left[\begin{array}{cccc|ccc} 0 & 0 & 0 & 0 & 1 & \frac{1}{4} & \frac{\sqrt{3}}{4} \\ -\frac{11}{127} & \frac{1}{4} & 0 & 0 & 1 & u_{11} & u_{23} \\ -\frac{2647}{72240} & \frac{1009}{1680} & \frac{1}{4} & 0 & 1 & -u_{22} & -u_{23} \\ -\frac{169}{1680} & \frac{113821}{283920} & \frac{473}{676} & 0 & 1 & -\frac{1}{4} & -\frac{\sqrt{3}}{4} \\ \hline -\frac{169}{3360} & \frac{1849}{3360} & \frac{1849}{3360} & -\frac{169}{3360} & 1 & 0 & 0 \\ -\frac{169}{1680} & -\frac{84839}{283920} & \frac{84839}{283920} & \frac{169}{1680} & 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ 0 & -\frac{43\sqrt{14595}}{35490} & \frac{43\sqrt{14595}}{35490} & 0 & 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{array}\right]$$

where $u_{22} = -\frac{1973}{29068} + \frac{2\sqrt{3}\sqrt{14595}}{7267}$ and $u_{23} = -\frac{1973\sqrt{3}}{29068} - \frac{2\sqrt{14595}}{7267}$. [1].

$G-$symplectic general linear method of order 4 is used to solve perturbed Kepler problem. G-symplectic methods with projection onto a single invariant manifold shows that the invariants H and L of the system are not conserved. But when we applied projection on both invariants with $G-$symplectic General Linear method the system remains conserved and shows good behavior as shown in Figure 3.17, Figure 3.18 and Figure 3.19.

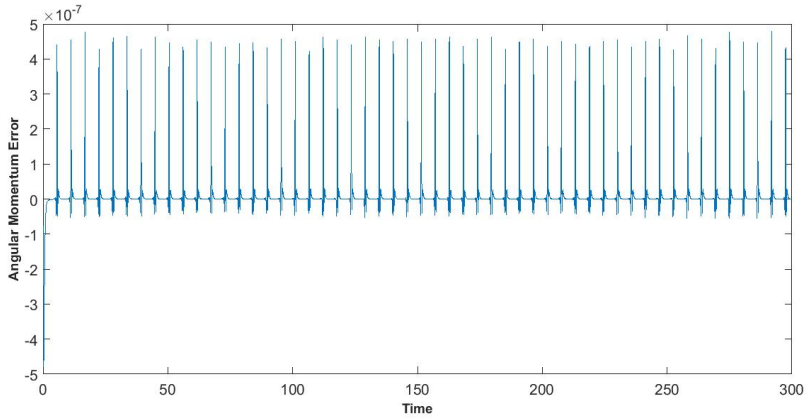

Figure 3.18: Results of G-symplectic GLM43 with projection on L as applied to the perturbed Kepler problem with step size $\triangle x = \frac{1}{100}$ and energy error $\triangle H$.

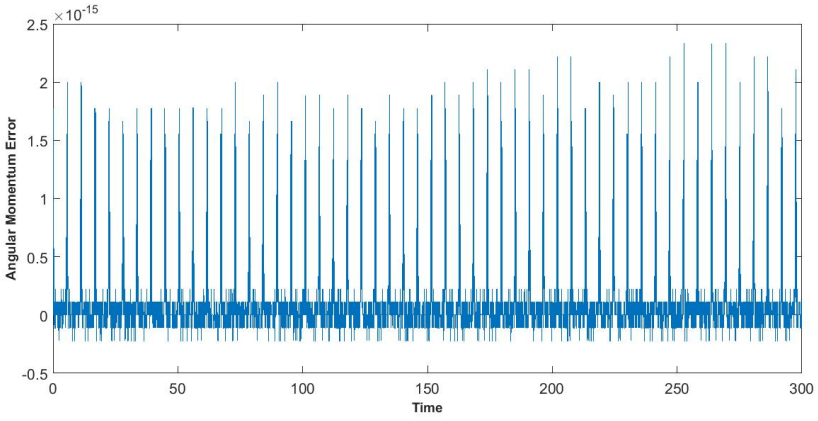

Figure 3.19: Result of G-symplectic GLM43 with projection on both invariants as applied to the perturbed Kepler problem with step size $\triangle x = \frac{1}{100}$ and the energy error $\triangle H$ plotted against it.

Chapter 4

Concluding Remarks

The present work presents a clear exposition of certain numerical methods. These methods are designed so as to account for the preservation of the quadratic invariants of the Hamiltonian mechanical systems represented by these differential models. The treatment of the subject has been made as self-contained as is possible for a work of this level. The preservation of the quadratic invariants of a Hamiltonian system is achieved using integrators from a populated class of numerical methods for systems of ODEs, collectively known as the general linear methods. In Chapter **1**, basic theory of differential equations, their classification, and some of the most well-known types which are frequently encountered in mathematical models for real-world problems hailing from variegated branches of science and technology is given and general systems of differential equations formally defined. The foundation for the study of numerical solutions of systems of ODEs is laid down in the general setting of not necessarily linear ODEs. As the subsequent part of the work is concerned only with systems of first-order linear ODEs, such systems are accorded special emphasis. Chapter 1 integrates fundamental concepts and serves as a kind of preamble to most of the following theory. It is advised that this chapter be perused frequently for a thorough understanding of the subsequent material. Definitions are, most of the time, laid out explicitly while other interesting ones are given using the bold text convention. If something important has been eluded, it is due to the limited scope of the present work. However, these apparent lacunae of exposition should cause no trouble to the keen readers who may supplement the exposition with standard reference works on the subject. The Hamiltonian system and its quadratic invariants are introduced in chapter **1**.

Chapter **2**, $G-$ symplectic general linear methods are discussed. The organized enquiry into the nature of different numerical methods culminates

in the development of the structure-preserving integrators for Hamiltonian systems. These methods are interesting because they respect the geometrically significant properties for these systems, such as symplecticity. Solutions to a differential system may be mathematically sound, but real-world restrictions on the problems have their own bias for adopting a solution as legitimate.

In Chapter **3**, various Hamiltonian systems are solved using a number of integrators introduced earlier to obtain valid solutions of the Hamiltonian equations of motions for these systems. A valid solution of a Hamiltonian system preserves some intrinsic properties of such systems whose conservation is desirable. It is illustrated using examples of Hamiltonian systems that the end results are rather unsatisfactory if methods without projection are used. The examples are then re-examined using the same methods bolstered by the accompanied projection technique and it is demonstrated that an excellent level of preservation of geometric invariants is achieved.

We have added the computations for the numerical methods in some detail within the present work so as to throw some light on the practical side of the subject as well. The theoretical exposition for numerical methods such as the one-step and the multi-step methods and the more comprehensive class of general linear methods is accompanied by illustrative specific cases such as the simple harmonic oscillator (systems with a single degree of freedom), and the perturbed Kepler problem (a system with more than one degree of freedom). In all these classical experimental problems, we arrived at the important result the energy of the Hamiltonian system is conserved with the application of the purpose-built general linear numerical methods armed with the useful projection technique. The same result for the energy conservation of the Hamiltonian system holds steadfast for the adaptive

class of numerical methods known as the canonical or symplectic methods.

In general, $G-$symplectic methods always keep the quadratic invariants of the system conserved without using any projection technique. We examine the perturbed Kepler problem which has two invariants. When $G-$symplectic method is applied, it gives us good preservation. If we apply the projection on H or L alone, the solution does not remain on the invariant manifold. On the other hand, if we apply the projection on both invariants, good preservation is achieved.

Bibliography

[1] Suris, Y.B. On the conservation of the symplectic structure in the numerical solution of Hamiltonian systems. *Numerical Solution of Ordinary Differential Equations*(1988).

[2] Lambert, J.D. *Numerical methods for ordinary differential systems: the initial-value problem (1991).*

[3] Sanz-Serna J.M. Symplectic integrators for Hamiltonian problems. *Acta Nu- mer.(1992).*

[4] Sanz-Serna, J.M, Calvo, M.P. Vol(7) of Applied Mathematics and Computational Mathematics *Numerical Hamiltonian Problems*, (1994).

[5] K. Feng. The step-transition operators for multi-step methods of ODEs, *J. Comput. Math* (1998).

[6] J.C. Butcher. General linear methods. *Acta Numerica* (2006).

[7] Hairer, E., Lubich, C. Wanner, G-Symplectic Integration of Hamiltonian Systems. In *Geometric numerical integration*, Springer, Berlin, Heidelberg. (2006)

[8] Habib, Y. . *Long-term behaviour of G-symplectic methods* (Doctoral dissertation, ResearchSpace@ Auckland).(2010)

[9] Butcher, J. C., Habib, Y., Hill, A. T., and Norton, T. J. *The control of parasitism in G-symplectic methods. SIAM Journal on Numerical Analysis.* (2014).

[10] Butcher, J. C. *Numerical methods for ordinary differential equations.* John Wiley and Sons. (2016).